



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:37 PM UTC

PDB ID : 6SZQ / pdb_00006szq
Title : Crystal structure of human DDAH-1
Authors : Hennig, S.; Vetter, I.R.; Schade, D.
Deposited on : 2019-10-02
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

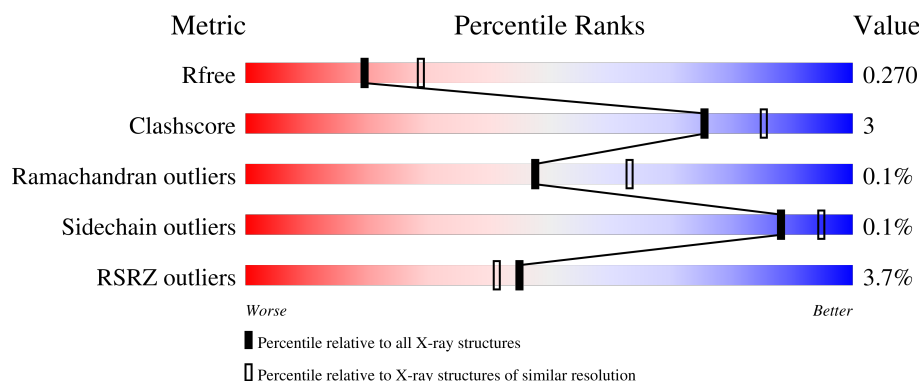
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	297	2% 85% 7% • 7%
1	B	297	% 86% 6% • 7%
1	C	297	3% 85% 10% 5%
1	D	297	5% 86% 10% •
1	E	297	3% 84% 12% 5%

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Mol	Chain	Length	Quality of chain
1	F	297	 7% 77% 14% .. 6%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13242 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called N(G),N(G)-dimethylarginine dimethylaminohydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2117	1329	367	407	14			
1	B	276	Total	C	N	O	S	0	0	0
			2117	1329	367	407	14			
1	C	281	Total	C	N	O	S	0	0	0
			2148	1348	374	412	14			
1	D	286	Total	C	N	O	S	0	0	0
			2183	1369	381	418	15			
1	E	283	Total	C	N	O	S	0	0	0
			2163	1358	376	414	15			
1	F	278	Total	C	N	O	S	0	0	0
			2134	1340	371	409	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP O94760
A	-10	ARG	-	expression tag	UNP O94760
A	-9	GLY	-	expression tag	UNP O94760
A	-8	SER	-	expression tag	UNP O94760
A	-7	HIS	-	expression tag	UNP O94760
A	-6	HIS	-	expression tag	UNP O94760
A	-5	HIS	-	expression tag	UNP O94760
A	-4	HIS	-	expression tag	UNP O94760
A	-3	HIS	-	expression tag	UNP O94760
A	-2	HIS	-	expression tag	UNP O94760
A	-1	GLY	-	expression tag	UNP O94760
A	0	SER	-	expression tag	UNP O94760
B	-11	MET	-	initiating methionine	UNP O94760
B	-10	ARG	-	expression tag	UNP O94760
B	-9	GLY	-	expression tag	UNP O94760
B	-8	SER	-	expression tag	UNP O94760
B	-7	HIS	-	expression tag	UNP O94760

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O94760
B	-5	HIS	-	expression tag	UNP O94760
B	-4	HIS	-	expression tag	UNP O94760
B	-3	HIS	-	expression tag	UNP O94760
B	-2	HIS	-	expression tag	UNP O94760
B	-1	GLY	-	expression tag	UNP O94760
B	0	SER	-	expression tag	UNP O94760
C	-11	MET	-	initiating methionine	UNP O94760
C	-10	ARG	-	expression tag	UNP O94760
C	-9	GLY	-	expression tag	UNP O94760
C	-8	SER	-	expression tag	UNP O94760
C	-7	HIS	-	expression tag	UNP O94760
C	-6	HIS	-	expression tag	UNP O94760
C	-5	HIS	-	expression tag	UNP O94760
C	-4	HIS	-	expression tag	UNP O94760
C	-3	HIS	-	expression tag	UNP O94760
C	-2	HIS	-	expression tag	UNP O94760
C	-1	GLY	-	expression tag	UNP O94760
C	0	SER	-	expression tag	UNP O94760
D	-11	MET	-	initiating methionine	UNP O94760
D	-10	ARG	-	expression tag	UNP O94760
D	-9	GLY	-	expression tag	UNP O94760
D	-8	SER	-	expression tag	UNP O94760
D	-7	HIS	-	expression tag	UNP O94760
D	-6	HIS	-	expression tag	UNP O94760
D	-5	HIS	-	expression tag	UNP O94760
D	-4	HIS	-	expression tag	UNP O94760
D	-3	HIS	-	expression tag	UNP O94760
D	-2	HIS	-	expression tag	UNP O94760
D	-1	GLY	-	expression tag	UNP O94760
D	0	SER	-	expression tag	UNP O94760
E	-11	MET	-	initiating methionine	UNP O94760
E	-10	ARG	-	expression tag	UNP O94760
E	-9	GLY	-	expression tag	UNP O94760
E	-8	SER	-	expression tag	UNP O94760
E	-7	HIS	-	expression tag	UNP O94760
E	-6	HIS	-	expression tag	UNP O94760
E	-5	HIS	-	expression tag	UNP O94760
E	-4	HIS	-	expression tag	UNP O94760
E	-3	HIS	-	expression tag	UNP O94760
E	-2	HIS	-	expression tag	UNP O94760
E	-1	GLY	-	expression tag	UNP O94760

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	UNP O94760
F	-11	MET	-	initiating methionine	UNP O94760
F	-10	ARG	-	expression tag	UNP O94760
F	-9	GLY	-	expression tag	UNP O94760
F	-8	SER	-	expression tag	UNP O94760
F	-7	HIS	-	expression tag	UNP O94760
F	-6	HIS	-	expression tag	UNP O94760
F	-5	HIS	-	expression tag	UNP O94760
F	-4	HIS	-	expression tag	UNP O94760
F	-3	HIS	-	expression tag	UNP O94760
F	-2	HIS	-	expression tag	UNP O94760
F	-1	GLY	-	expression tag	UNP O94760
F	0	SER	-	expression tag	UNP O94760

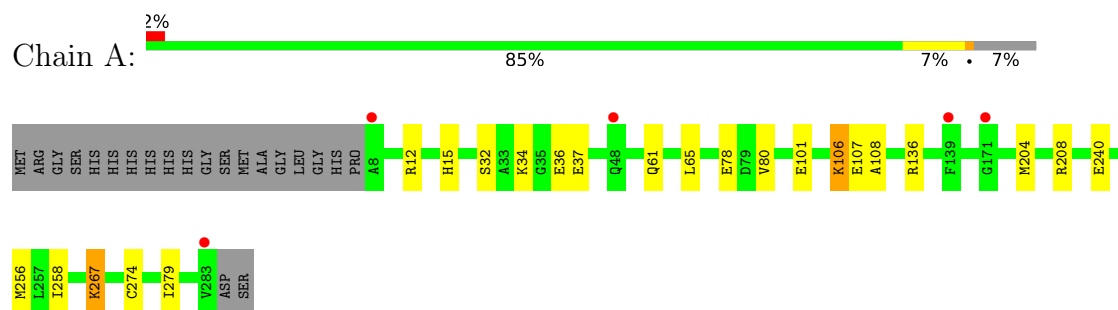
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	69	Total O 69 69	0	0
2	B	71	Total O 71 71	0	0
2	C	96	Total O 96 96	0	0
2	D	44	Total O 44 44	0	0
2	E	59	Total O 59 59	0	0
2	F	41	Total O 41 41	0	0

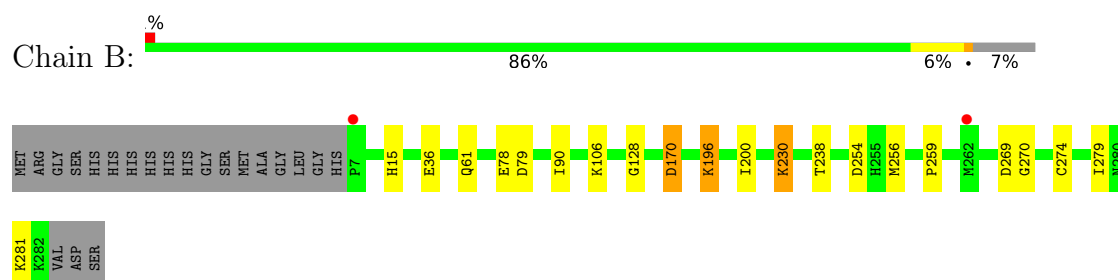
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

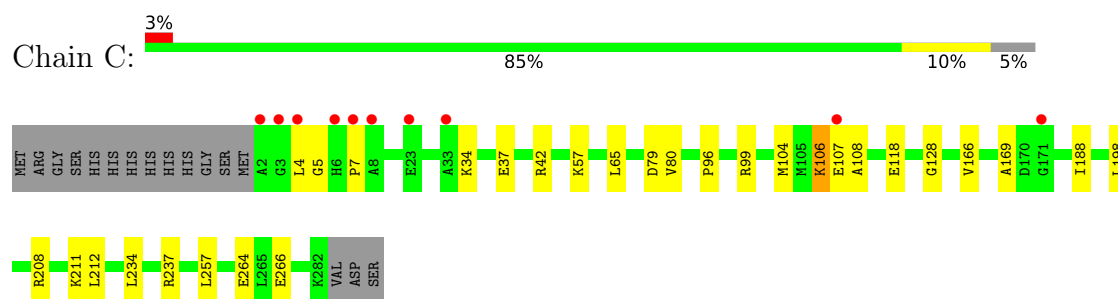
- Molecule 1: N(G),N(G)-dimethylarginine dimethylaminohydrolase 1



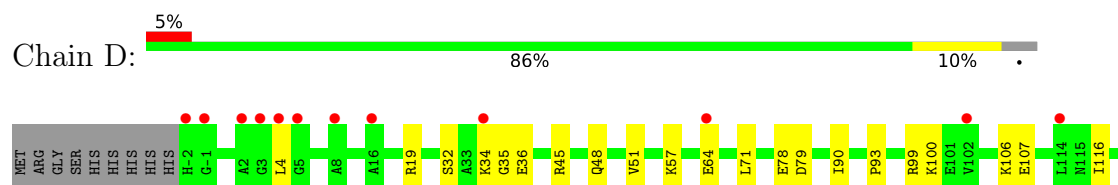
- Molecule 1: N(G),N(G)-dimethylarginine dimethylaminohydrolase 1

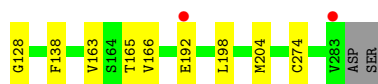


- Molecule 1: N(G),N(G)-dimethylarginine dimethylaminohydrolase 1

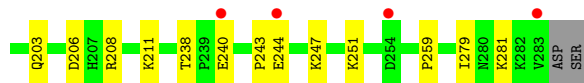
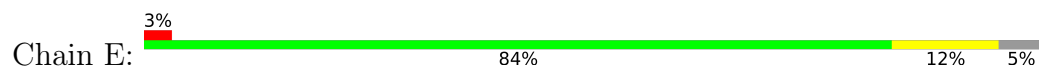


- Molecule 1: N(G),N(G)-dimethylarginine dimethylaminohydrolase 1

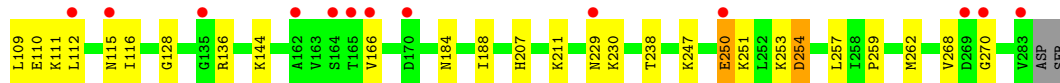
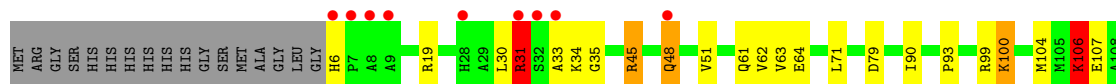
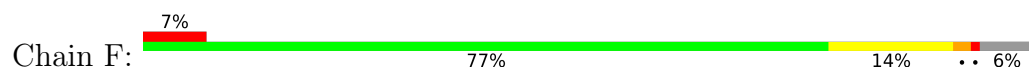




- Molecule 1: N(G),N(G)-dimethylarginine dimethylaminohydrolase 1



- Molecule 1: N(G),N(G)-dimethylarginine dimethylaminohydrolase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.15Å 76.15Å 116.84Å 90.00° 95.47° 90.00°	Depositor
Resolution (Å)	46.65 – 2.41 46.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.65-2.41) 99.5 (46.65-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.223 , 0.270 0.224 , 0.270	Depositor DCC
R_{free} test set	2100 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13242	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6580e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	1/2149 (0.0%)	1.05	12/2904 (0.4%)
1	B	0.69	3/2150 (0.1%)	1.03	10/2905 (0.3%)
1	C	0.66	2/2182 (0.1%)	1.01	11/2949 (0.4%)
1	D	0.76	4/2218 (0.2%)	1.12	20/2997 (0.7%)
1	E	0.77	1/2197 (0.0%)	1.26	30/2969 (1.0%)
1	F	0.99	7/2168 (0.3%)	1.35	34/2931 (1.2%)
All	All	0.76	18/13064 (0.1%)	1.14	117/17655 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	F	0	6
All	All	0	10

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	VAL	CA-C	16.17	1.69	1.52
1	F	270	GLY	CA-C	-14.77	1.41	1.52
1	D	166	VAL	CA-C	13.22	1.66	1.52
1	B	269	ASP	C-N	-10.96	1.28	1.33
1	B	270	GLY	CA-C	-9.05	1.44	1.51
1	D	165	THR	C-N	7.65	1.42	1.33
1	C	166	VAL	CA-C	6.72	1.57	1.52
1	A	107	GLU	CD-OE1	6.63	1.38	1.25
1	F	107	GLU	N-CA	6.18	1.53	1.46
1	F	45	ARG	CD-NE	6.08	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	110	GLU	CD-OE1	-5.87	1.14	1.25
1	C	4	LEU	CG-CD1	-5.78	1.33	1.52
1	F	166	VAL	C-O	-5.67	1.17	1.24
1	D	166	VAL	N-CA	-5.61	1.39	1.46
1	F	107	GLU	CA-CB	5.60	1.62	1.53
1	B	230	LYS	CG-CD	5.58	1.69	1.52
1	D	166	VAL	C-N	-5.52	1.27	1.33
1	E	281	LYS	CB-CG	-5.16	1.36	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	GLN	CB-CG-CD	13.82	136.10	112.60
1	D	48	GLN	CA-CB-CG	13.18	140.45	114.10
1	A	34	LYS	CB-CG-CD	12.07	139.06	111.30
1	F	48	GLN	N-CA-CB	11.46	129.08	110.40
1	E	208	ARG	CB-CG-CD	-10.31	87.59	111.30
1	D	198	LEU	CB-CG-CD2	-9.95	80.85	110.70
1	B	254	ASP	CB-CA-C	-9.69	90.62	110.38
1	C	4	LEU	CA-CB-CG	9.49	149.53	116.30
1	D	45	ARG	NE-CZ-NH2	9.43	127.69	119.20
1	C	37	GLU	CA-CB-CG	-9.15	95.79	114.10
1	B	196	LYS	CG-CD-CE	-8.73	91.22	111.30
1	D	48	GLN	CB-CA-C	-8.60	94.16	110.67
1	E	23	GLU	CA-CB-CG	8.48	131.05	114.10
1	E	203	GLN	CA-CB-CG	8.33	130.77	114.10
1	F	253	LYS	CB-CA-C	-8.32	92.61	109.99
1	E	34	LYS	CA-CB-CG	8.24	130.57	114.10
1	A	34	LYS	CG-CD-CE	-8.21	92.41	111.30
1	F	48	GLN	CA-CB-CG	8.08	130.25	114.10
1	E	106	LYS	CA-C-N	8.00	131.34	120.38
1	E	106	LYS	C-N-CA	8.00	131.34	120.38
1	C	107	GLU	CA-CB-CG	7.63	129.36	114.10
1	F	111	LYS	CA-CB-CG	7.62	129.34	114.10
1	F	166	VAL	O-C-N	7.56	129.72	121.10
1	F	31	ARG	CA-C-N	7.46	131.65	120.31
1	F	31	ARG	C-N-CA	7.46	131.65	120.31
1	E	34	LYS	CB-CG-CD	-7.42	94.25	111.30
1	F	109	LEU	CA-CB-CG	7.37	142.11	116.30
1	F	100	LYS	N-CA-CB	-7.23	99.75	110.53
1	F	34	LYS	CG-CD-CE	-7.22	94.69	111.30
1	E	144	LYS	CG-CD-CE	-7.21	94.71	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	208	ARG	N-CA-CB	-7.16	98.55	110.37
1	F	247	LYS	CD-CE-NZ	-7.16	88.98	111.90
1	F	253	LYS	CB-CG-CD	-7.00	95.21	111.30
1	C	208	ARG	CG-CD-NE	-6.91	96.79	112.00
1	E	144	LYS	CD-CE-NZ	6.87	133.88	111.90
1	F	253	LYS	CA-CB-CG	6.82	127.74	114.10
1	F	270	GLY	O-C-N	-6.78	117.57	123.80
1	D	32	SER	CB-CA-C	6.74	123.24	109.55
1	A	107	GLU	CG-CD-OE2	-6.69	103.00	118.40
1	F	262	MET	CG-SD-CE	-6.66	86.26	100.90
1	F	254	ASP	N-CA-CB	-6.59	99.66	110.40
1	B	170	ASP	N-CA-C	6.57	124.78	110.80
1	E	203	GLN	CB-CG-CD	-6.51	101.53	112.60
1	F	110	GLU	CA-CB-CG	6.47	127.05	114.10
1	E	136	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	E	281	LYS	CB-CG-CD	-6.35	96.70	111.30
1	A	136	ARG	CB-CG-CD	6.34	125.88	111.30
1	D	34	LYS	CG-CD-CE	6.34	125.88	111.30
1	F	268	VAL	CA-C-N	6.34	131.82	122.82
1	F	268	VAL	C-N-CA	6.34	131.82	122.82
1	F	115	ASN	CB-CA-C	-6.29	99.82	109.89
1	F	48	GLN	CB-CA-C	-6.27	96.89	109.99
1	B	270	GLY	O-C-N	-6.25	119.42	123.35
1	C	80	VAL	N-CA-CB	-6.22	102.62	112.07
1	E	240	GLU	CA-CB-CG	-6.09	101.92	114.10
1	A	208	ARG	CB-CG-CD	6.07	125.27	111.30
1	B	196	LYS	CB-CG-CD	6.07	125.26	111.30
1	D	36	GLU	CB-CG-CD	-6.04	102.34	112.60
1	A	136	ARG	CA-CB-CG	6.03	126.15	114.10
1	E	107	GLU	CA-CB-CG	6.02	126.13	114.10
1	F	100	LYS	CB-CA-C	6.00	120.10	109.65
1	D	36	GLU	N-CA-C	5.99	119.27	110.59
1	D	45	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	B	281	LYS	CG-CD-CE	5.97	125.04	111.30
1	E	144	LYS	N-CA-CB	-5.97	101.11	110.30
1	A	107	GLU	N-CA-CB	-5.96	101.36	110.12
1	D	57	LYS	CB-CA-C	5.96	119.66	109.24
1	D	106	LYS	CA-C-N	5.87	128.14	120.28
1	D	106	LYS	C-N-CA	5.87	128.14	120.28
1	C	106	LYS	CA-C-N	5.86	128.46	120.54
1	C	106	LYS	C-N-CA	5.86	128.46	120.54
1	D	4	LEU	CA-CB-CG	5.84	136.76	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	247	LYS	CB-CA-C	-5.81	99.52	110.67
1	D	107	GLU	CA-CB-CG	5.81	125.71	114.10
1	A	32	SER	CB-CA-C	-5.79	101.75	110.90
1	C	57	LYS	CA-CB-CG	5.79	125.68	114.10
1	E	44	GLU	N-CA-CB	5.77	119.19	110.30
1	F	115	ASN	N-CA-CB	5.76	118.43	109.85
1	C	169	ALA	CA-C-N	5.74	132.50	121.54
1	C	169	ALA	C-N-CA	5.74	132.50	121.54
1	F	229	ASN	CA-CB-CG	5.68	118.28	112.60
1	B	196	LYS	CB-CA-C	-5.67	101.38	110.79
1	E	107	GLU	CB-CG-CD	-5.56	103.14	112.60
1	A	267	LYS	CD-CE-NZ	5.56	129.69	111.90
1	D	64	GLU	CG-CD-OE2	-5.55	105.63	118.40
1	E	243	PRO	CA-C-N	5.52	128.70	120.31
1	E	243	PRO	C-N-CA	5.52	128.70	120.31
1	E	34	LYS	N-CA-CB	-5.51	102.65	110.58
1	E	105	MET	CA-C-N	5.50	127.92	120.65
1	E	105	MET	C-N-CA	5.50	127.92	120.65
1	A	240	GLU	CB-CG-CD	5.48	121.92	112.60
1	F	253	LYS	CD-CE-NZ	5.44	129.31	111.90
1	B	36	GLU	CB-CG-CD	-5.43	103.37	112.60
1	E	114	LEU	CA-CB-CG	5.43	135.29	116.30
1	C	4	LEU	CD1-CG-CD2	-5.39	98.94	110.80
1	F	106	LYS	CA-C-N	5.39	127.81	120.54
1	F	106	LYS	C-N-CA	5.39	127.81	120.54
1	E	244	GLU	CB-CG-CD	-5.39	103.44	112.60
1	F	61	GLN	CB-CG-CD	5.35	121.70	112.60
1	F	144	LYS	CG-CD-CE	5.35	123.60	111.30
1	B	254	ASP	N-CA-CB	5.34	118.52	110.30
1	B	230	LYS	CA-CB-CG	5.32	124.73	114.10
1	E	23	GLU	CB-CG-CD	5.30	121.62	112.60
1	E	85	GLU	CA-CB-CG	5.28	124.65	114.10
1	D	166	VAL	O-C-N	5.23	127.06	121.10
1	E	34	LYS	CD-CE-NZ	-5.23	95.16	111.90
1	D	192	GLU	CB-CG-CD	5.22	121.48	112.60
1	A	106	LYS	CA-C-N	5.18	127.22	120.28
1	A	106	LYS	C-N-CA	5.18	127.22	120.28
1	F	229	ASN	CB-CA-C	5.17	120.71	110.42
1	F	253	LYS	CA-C-N	5.12	130.11	121.14
1	F	253	LYS	C-N-CA	5.12	130.11	121.14
1	F	251	LYS	CD-CE-NZ	5.12	128.28	111.90
1	D	166	VAL	CA-C-O	-5.12	113.09	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	30	LEU	CA-CB-CG	5.08	134.08	116.30
1	E	159	LYS	N-CA-CB	-5.06	102.15	110.40
1	D	51	VAL	N-CA-CB	-5.00	103.08	110.58

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	GLN	Sidechain
1	B	61	GLN	Sidechain
1	C	5	GLY	Peptide
1	C	7	PRO	Peptide
1	F	106	LYS	Mainchain
1	F	250	GLU	Sidechain,Peptide
1	F	35	GLY	Peptide
1	F	6	HIS	Peptide
1	F	64	GLU	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2117	0	2148	14	0
1	B	2117	0	2147	8	0
1	C	2148	0	2175	12	0
1	D	2183	0	2211	9	0
1	E	2163	0	2196	11	0
1	F	2134	0	2162	25	0
2	A	69	0	0	0	0
2	B	71	0	0	1	0
2	C	96	0	0	0	0
2	D	44	0	0	1	0
2	E	59	0	0	0	0
2	F	41	0	0	1	0
All	All	13242	0	13039	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:GLU:OE2	1:F:257:LEU:HD13	1.67	0.93
1:A:12:ARG:NH2	1:E:206:ASP:OD2	2.05	0.89
1:F:45:ARG:HD2	1:F:48:GLN:HE22	1.36	0.89
1:F:90:ILE:HD12	1:F:116:ILE:HG23	1.73	0.71
1:A:12:ARG:HH22	1:E:206:ASP:CG	1.98	0.70
1:F:136:ARG:HH12	1:F:184:ASN:ND2	1.90	0.70
1:D:90:ILE:HD12	1:D:116:ILE:HG23	1.76	0.68
1:F:136:ARG:NH1	1:F:207:HIS:CD2	2.63	0.67
1:C:106:LYS:NZ	1:C:118:GLU:OE2	2.29	0.66
1:F:19:ARG:NH2	1:F:104:MET:HE3	2.11	0.65
1:E:198:LEU:HD21	1:E:211:LYS:HD2	1.84	0.59
1:D:71:LEU:HD11	1:D:100:LYS:HB2	1.87	0.57
1:F:45:ARG:CD	1:F:48:GLN:HE22	2.14	0.56
1:B:196:LYS:HE3	1:B:200:ILE:HD11	1.86	0.56
1:B:230:LYS:NZ	1:B:256:MET:SD	2.71	0.56
1:C:198:LEU:HD21	1:C:211:LYS:HD2	1.87	0.55
1:F:93:PRO:HD2	1:F:99:ARG:HG2	1.89	0.54
1:E:15:HIS:HB2	1:E:279:ILE:HB	1.91	0.52
1:A:36:GLU:CB	1:A:267:LYS:HZ3	2.23	0.52
1:F:136:ARG:CZ	1:F:207:HIS:CD2	2.94	0.51
1:F:45:ARG:NH1	1:F:48:GLN:NE2	2.59	0.50
1:A:15:HIS:HB2	1:A:279:ILE:HB	1.92	0.50
1:C:65:LEU:HD22	1:C:104:MET:HG3	1.94	0.49
1:E:138:PHE:HB2	1:E:163:VAL:HG22	1.94	0.49
1:A:36:GLU:CB	1:A:267:LYS:NZ	2.76	0.49
1:F:136:ARG:CZ	1:F:207:HIS:NE2	2.76	0.48
1:F:71:LEU:HD21	1:F:100:LYS:HD3	1.94	0.48
1:C:237:ARG:NH2	1:C:266:GLU:OE1	2.46	0.48
1:F:188:ILE:HG21	1:F:211:LYS:HE2	1.95	0.48
1:F:31:ARG:HG2	1:F:33:ALA:H	1.79	0.48
1:C:65:LEU:HD21	1:C:108:ALA:HB2	1.96	0.47
1:F:45:ARG:HD2	1:F:48:GLN:NE2	2.17	0.47
1:F:63:VAL:HG21	1:F:112:LEU:HD11	1.97	0.47
1:C:188:ILE:HG12	1:C:198:LEU:HD22	1.96	0.47
1:E:93:PRO:HD2	1:E:99:ARG:HG2	1.96	0.47
1:A:36:GLU:HB3	1:A:267:LYS:NZ	2.30	0.46
1:D:138:PHE:HB2	1:D:163:VAL:HG22	1.97	0.46
1:C:234:LEU:HB3	1:C:257:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:ILE:HD13	1:F:106:LYS:HB2	1.98	0.46
1:C:79:ASP:HA	1:C:128:GLY:H	1.81	0.45
1:A:37:GLU:O	1:A:267:LYS:NZ	2.49	0.45
1:C:42:ARG:HB3	1:C:264:GLU:HG3	1.98	0.45
1:E:238:THR:HG22	1:E:259:PRO:HB2	1.99	0.45
1:C:96:PRO:HA	1:C:99:ARG:HG3	1.99	0.45
1:D:93:PRO:HD2	1:D:99:ARG:HG3	1.98	0.45
1:F:79:ASP:HA	1:F:128:GLY:H	1.82	0.45
1:F:136:ARG:HH12	1:F:184:ASN:HD22	1.64	0.45
1:F:254:ASP:OD1	1:F:254:ASP:N	2.46	0.45
1:B:79:ASP:HA	1:B:128:GLY:H	1.82	0.44
1:E:188:ILE:HG12	1:E:198:LEU:HD22	1.99	0.44
1:F:51:VAL:HG13	1:F:62:VAL:HG11	1.98	0.44
1:F:230:LYS:NZ	2:F:308:HOH:O	2.50	0.43
1:F:250:GLU:CD	1:F:257:LEU:HD13	2.40	0.43
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.94	0.43
1:B:78:GLU:HB3	1:B:274:CYS:HA	1.99	0.42
1:A:106:LYS:HE2	1:A:106:LYS:HB3	1.89	0.42
1:A:256:MET:HE3	1:A:258:ILE:HD11	2.01	0.42
1:D:79:ASP:HA	1:D:128:GLY:H	1.85	0.42
1:A:78:GLU:HB3	1:A:274:CYS:HA	2.01	0.42
1:B:90:ILE:HG13	1:B:106:LYS:HG3	2.01	0.42
1:F:45:ARG:CZ	1:F:48:GLN:NE2	2.83	0.42
1:B:15:HIS:HB2	1:B:279:ILE:HB	2.02	0.42
1:A:65:LEU:HD21	1:A:108:ALA:HB2	2.01	0.42
1:D:19:ARG:NH1	2:D:304:HOH:O	2.50	0.42
1:D:78:GLU:HB3	1:D:274:CYS:HA	2.02	0.41
1:C:34:LYS:HD3	1:C:34:LYS:HA	1.76	0.41
1:B:230:LYS:NZ	2:B:310:HOH:O	2.52	0.41
1:D:204:MET:HE3	1:D:204:MET:HB2	1.93	0.41
1:D:90:ILE:CD1	1:D:116:ILE:HG23	2.48	0.41
1:E:180:MET:SD	1:E:186:ILE:HD13	2.61	0.41
1:F:238:THR:HG22	1:F:259:PRO:HB2	2.02	0.41
1:A:36:GLU:HB2	1:A:267:LYS:NZ	2.36	0.40
1:E:251:LYS:HD3	1:E:251:LYS:HA	1.92	0.40
1:A:80:VAL:HG11	1:A:101:GLU:HB2	2.03	0.40
1:A:204:MET:HE3	1:A:204:MET:HB2	1.93	0.40
1:B:238:THR:HG22	1:B:259:PRO:HB2	2.02	0.40
1:E:181:ALA:HB2	1:E:187:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/297 (92%)	267 (97%)	7 (3%)	0	100	100
1	B	274/297 (92%)	266 (97%)	7 (3%)	1 (0%)	30	42
1	C	279/297 (94%)	269 (96%)	10 (4%)	0	100	100
1	D	284/297 (96%)	274 (96%)	9 (3%)	1 (0%)	30	42
1	E	281/297 (95%)	274 (98%)	7 (2%)	0	100	100
1	F	276/297 (93%)	265 (96%)	11 (4%)	0	100	100
All	All	1668/1782 (94%)	1615 (97%)	51 (3%)	2 (0%)	48	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ASP
1	D	35	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/249 (94%)	233 (100%)	0	100	100
1	B	233/249 (94%)	233 (100%)	0	100	100
1	C	235/249 (94%)	235 (100%)	0	100	100
1	D	239/249 (96%)	239 (100%)	0	100	100
1	E	237/249 (95%)	237 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	235/249 (94%)	234 (100%)	1 (0%)	84	92
All	All	1412/1494 (94%)	1411 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	31	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	115	ASN
1	A	195	GLN
1	B	115	ASN
1	C	27	GLN
1	D	6	HIS
1	D	48	GLN
1	E	61	GLN
1	F	28	HIS
1	F	48	GLN
1	F	184	ASN
1	F	226	ASN
1	F	229	ASN
1	F	232	HIS
1	F	255	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/297 (92%)	0.28	5 (1%) 67 64	29, 42, 65, 82	0
1	B	276/297 (92%)	0.19	2 (0%) 84 82	29, 42, 63, 74	0
1	C	281/297 (94%)	0.30	10 (3%) 46 42	26, 40, 64, 92	0
1	D	286/297 (96%)	0.59	14 (4%) 35 31	33, 52, 76, 88	0
1	E	283/297 (95%)	0.35	9 (3%) 50 47	31, 45, 71, 91	0
1	F	278/297 (93%)	0.78	22 (7%) 18 15	36, 56, 81, 93	0
All	All	1680/1782 (94%)	0.42	62 (3%) 45 41	26, 46, 73, 93	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ALA	4.4
1	D	4	LEU	4.3
1	C	6	HIS	4.2
1	D	3	GLY	4.1
1	F	6	HIS	3.7
1	D	5	GLY	3.7
1	C	8	ALA	3.6
1	C	3	GLY	3.5
1	D	283	VAL	3.5
1	E	3	GLY	3.4
1	D	-1	GLY	3.3
1	B	7	PRO	3.3
1	F	164	SER	3.2
1	C	4	LEU	3.2
1	C	7	PRO	3.2
1	C	2	ALA	3.1
1	F	7	PRO	3.1
1	F	32	SER	3.1
1	E	5	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	48	GLN	2.9
1	D	64	GLU	2.9
1	A	283	VAL	2.8
1	A	171	GLY	2.8
1	F	33	ALA	2.8
1	E	7	PRO	2.8
1	C	107	GLU	2.7
1	F	162	ALA	2.7
1	F	270	GLY	2.7
1	C	171	GLY	2.6
1	F	31	ARG	2.6
1	C	23	GLU	2.6
1	F	170	ASP	2.5
1	E	254	ASP	2.5
1	F	250	GLU	2.5
1	F	9	ALA	2.4
1	F	283	VAL	2.4
1	E	6	HIS	2.4
1	A	48	GLN	2.3
1	C	33	ALA	2.3
1	D	-2	HIS	2.3
1	A	8	ALA	2.3
1	D	8	ALA	2.3
1	F	28	HIS	2.2
1	E	244	GLU	2.2
1	E	110	GLU	2.2
1	F	135	GLY	2.2
1	F	269	ASP	2.2
1	E	283	VAL	2.1
1	F	166	VAL	2.1
1	D	192	GLU	2.1
1	E	240	GLU	2.1
1	B	262	MET	2.1
1	D	16	ALA	2.1
1	F	229	ASN	2.1
1	D	34	LYS	2.1
1	A	139	PHE	2.1
1	D	102	VAL	2.1
1	D	114	LEU	2.1
1	F	165	THR	2.1
1	F	8	ALA	2.0
1	F	115	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	112	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.